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Abstract

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Keywords:

1. Introduction

Suppose $X_1, \dots, X_n$ are i.i.d. from $N_p(\mu_X, \Sigma_X)$, where $X_i \in \mathbb{R}^p$. We denote $X = (X_1, \dots, X_n)$. In this paper, we assume $n < p$.

Consider a linear regression model $y = \beta_0 \mathbf{1}_n + X^T\beta + \epsilon$, where $\mathbf{1}_n$ is n dimensional vector with all elements equal to 1 and ϵ has distribution $N(0, \sigma^2 I_n)$.

Let $\Sigma_X = P\Lambda P^T$ be the spectral decomposition of Σ_X, where $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_p)$ with $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p$ and P is an orthogonal matrix. In PCA context, it is assumed that Σ_X is spiked, that is $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r > \lambda_{r+1} = \dots = \lambda_p$ for some $r > 0$ (See [1]). Denote by P_1 the first r column of P and P_2 the last $p - r$ column of P. The aim of PCA is to estimate P_1. In this paper, we allow Σ_X to be either spiked or non-spiked. Non-spike means that there's no principal component ($r = 0$). That is, $\lambda_1 = \dots = \lambda_p$. Spike means that there's r principal components for $r > 0$. In either case, let $\lambda = \lambda_{r+1} = \dots = \lambda_p$.

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[1]Since 1880.

If Σ_X is indeed spiked,

$$y = \beta_0 \mathbf{1}_n + X^T P_1 P_1^T \beta + X^T P_2 P_2^T \beta + \epsilon, \tag{1}$$

where $X^T P_1$ and $X^T P_2$ are independent. PCR try to do regression between y and $X^T P_1$. Since P_1 is not observed, it is substituted by an estimator $\tilde{P}_1$. Traditionally, PCR is a technique for analyzing multiple regression data that suffers from multicollinearity. Recently, PCR is a practical method to deal with high dimensional regression. If $p < n$, the full multicollinearity phenomenon shows up even if predictors are independent. It calls for a test procedure to justify the appropriateness of PCR. To be precise, we consider testing the hypotheses

$$H : \Sigma \text{ is non-spiked or } \Sigma \text{ is spiked and } P_1^T \beta = 0 \tag{2}$$

versus

$$K : \Sigma \text{ is spiked and } P_1^T \beta \neq 0. \tag{3}$$

If P_1 is observed, then the problem is reduced to testing an ordinary regression model. However, it's not the case. In fact, the classical F-test statistic for the regression between y and $X^T \tilde{P}_1$ may not be a good choice for at least three reasons:

1. From equation

   $$y = \beta_0 \mathbf{1}_n + X^T \tilde{P}_1 \tilde{P}_1^T \beta + X^T (I_p - \tilde{P}_1 \tilde{P}_1^T) \beta + \epsilon, \tag{4}$$

   we can see that the F-test suffers from Endogeneity.
2. The estimator of P_1 may not be consistent in high dimension. Moreover, Σ_X may not be spiked and, as a result, there's no principal component.
3. Even if there's additional information or data to estimate P_1, we will never know weather we estimate P_1 well enough such that the F-test is valid.

[2] proposed a generalized likelihood ratio test (GLRT) for testing high dimensional mean values. Roughly speaking, GLRT projects data to lower dimension by a direction a such that likelihood ratio is maximized. GLRT is likelihood

based, it can be regarded as a generalization of classical LRT in high dimension setting.

In this paper we apply the GLRT method to the problem of testing the significance of PCR.

2. New Test

It can be seen that $(X_1^T, y_1)^T, \ldots, (X_n^T, y_n)^T$ are i.i.d. from $N_{p+1}(\mu, \Sigma)$, where $\mu = (\mu_X^T, \beta_0)^T$ and

$$\Sigma = \begin{pmatrix} \Sigma_X & \Sigma_X \beta \\ \beta^T \Sigma_X & \beta^T \Sigma_X \beta + \sigma^2 \end{pmatrix}. \tag{5}$$

Denote $\Theta : (\mu, \Sigma)$. Define the hypothesis H_a by

$$H_a : \mathrm{Cov}(a^T X_i, y_i) = 0, \tag{6}$$

where $a \in \mathbb{R}^p$ and $a^T a = 1$. Let

$$S = \frac{1}{n} \sum_{i=1}^{n} \begin{pmatrix} (X_i - \bar{X})(X_i - \bar{X})^T & (X_i - \bar{X})(y_i - \bar{y})^T \\ (y_i - \bar{y})(X_i - \bar{X})^T & (y_i - \bar{y})(y_i - \bar{y})^T \end{pmatrix} = \begin{pmatrix} S_{XX} & S_{Xy} \\ S_{yX} & S_{yy} \end{pmatrix}, \tag{7}$$

and

$$S_a = \begin{pmatrix} a^T & 0 \\ 0 & 1 \end{pmatrix} S \begin{pmatrix} a & 0 \\ 0 & 1 \end{pmatrix}, \Sigma_a = \begin{pmatrix} a^T & 0 \\ 0 & 1 \end{pmatrix} \Sigma \begin{pmatrix} a & 0 \\ 0 & 1 \end{pmatrix}. \tag{8}$$

The likelihood function of $(a^T X_i, y_i)$, $i = 1, \ldots, n$, is

$$L_a(\theta; X, Y) = (2\pi)^{-n} |\Sigma_a|^{-n/2} \exp\left(-\frac{1}{2} \mathrm{tr} \Sigma_a^{-1} S_a\right). \tag{9}$$

Then the maximum likelihood is

$$L(a) = \sup_{\theta \in \Theta} L_a(\theta; X, Y) = (2\pi)^{-n} |S_a|^{-n/2} e^{-n}. \tag{10}$$

If $|S_a| = 0$, then 10 is interpreted as $+\infty$. Similarly, the maximum likelihood under H_a is

$$L(a) = \sup_{\theta \in H} L_a(\theta; X, Y) = (2\pi)^{-n} |a^T S_{XX} a S_{yy}|^{-n/2} e^{-n}. \tag{11}$$

In [2], GLRT is defined as

$$\min_{L(a)=+\infty} L_H(a) \quad s.t. \quad a^T a = 1. \tag{12}$$

The idea of GLRT is to find a such that $L(a) = +\infty$ and $L_H(a) < +\infty$ as small as possible such that the discrepancy between the likelihood values $L(a)$ and $L_H(a)$ is maximized. We call the direction a^* obtained by (12) the GLRT direction.

From the expression of $L(a)$ and $L_H(a)$, a^* is equal to

$$a^* = \text{argmax}_{a^T a=1} a^T S_{XX} a \quad s.t. \quad |S_a| = 0. \tag{13}$$

Such a direction a^* can be expected to make $|\Sigma_a|$ small and $a^T \Sigma_{XX} a$ large. That is, the variance of $a^T X_i$ is large and $a^T X_i$ and y_i are highly correlated. If X_i has certain principal components which are correlated to y_i, the direction a^* is expected to be close to corresponding principal directions.

Next we solve the optimization problem (13). Let $Q_n = I_n - \frac{1}{n}\mathbf{1}_n\mathbf{1}_n^T$. Denote by $Q_n = WW^T$ the rank decomposition of Q_n, where W_n is an $n \times (n-1)$ matrix with $W^T W = I_{n-1}$. Then $|S_a| = 0$ is equivalent to $a^T XQX^T a y^T Qy = (a^T XQy)^2$ and is equivalent to $W^T X^T a = W^T yk$ for some $k \in \mathbb{R}$. It follows that

$$a = XW(W^T X^T XW)^{-1} W^T yk + (I - XW(W^T X^T XW)^{-1} W^T X^T)a. \tag{14}$$

Since $a^T a = 1$,

$$k^2 y^T W(W^T X^T XW)^{-1} W^T y + a^T (I - XW(W^T X^T XW)^{-1} W^T X^T)a = 1. \tag{15}$$

Note that

$$L_H(a) \propto (a^T XQX^T a y^T Qy)^{-n/2} = \left(k^2 (y^T Q_n y)^2\right)^{-n/2}. \tag{16}$$

To make $L_H(a)$ minimized, we should maximize k^2. So the second term of 15 should be 0. That is

$$a = XW(W^T X^T XW)^{-1} W^T yk \tag{17}$$

Hence

$$k^2 = \frac{1}{y^T W (W^T X^T X W)^{-1} W^T y}, \tag{18}$$

and

$$L_H(a) \propto (a^T X Q X^T a y^T Q y)^{-n/2} = \left(\frac{(y^T Q_n y)^2}{y^T W (W^T X^T X W)^{-1} W^T y} \right)^{-n/2}. \tag{19}$$

After homogenization, we define

$$T = \frac{y^T Q_n y}{y^T W (W^T X^T X W)^{-1} W^T y}.$$

If T is large, we reject H.

3. Main Results

Let $\tilde{y} = W^T y$, $\tilde{X} = XW$, $\tilde{\epsilon} = W^T \epsilon$. Then the columns of $\tilde{X}$ are i.i.d. distributed as $N(0, \Sigma_X)$, $\tilde{\epsilon} \sim N(0, \sigma^2 I_{n-1})$ and $\tilde{y} = \tilde{X}^T \beta + \tilde{\epsilon}$. The test statistic can be written as

$$T = \frac{\tilde{y}^T \tilde{y}}{\tilde{y}^T (\tilde{X}^T \tilde{X})^{-1} \tilde{y}}.$$

The null hypotheses H is the union of two disjoint hypothesis $H = \cup_{i=1}^2 H_i$, where H_1: There's no principal component and H_2: There's r principal components with $r > 0$ and $P_1^T \beta = 0$. We have the following theorem

Theorem 1. *Suppose $p/n \to \infty$ and H_1 is true. Then*

- *If $\|\beta\|^2 \to 0$ or $\|\beta\|^2 \to +\infty$, then*

$$T/(\lambda p) \xrightarrow{P} 1. \tag{20}$$

- *If $\sqrt{p}\|\beta\|^2 \to 0$ and $\frac{p}{n}\|\beta\|^2 \to 0$, then*

$$\frac{T - \lambda(p - n + 2)}{\lambda\sqrt{2(p - n + 2)}} \xrightarrow{\mathcal{L}} N(0, 1). \tag{21}$$

- *If $\frac{n}{p}\|\beta\|^2 \to \infty$ and $\frac{1}{\sqrt{p}}\|\beta\|^2 \to \infty$, then*

$$\frac{T - \lambda p}{\lambda\sqrt{2p}} \xrightarrow{\mathcal{L}} N(0, 1). \tag{22}$$

4. Appendix

For random variable ξ and η, we write $\xi \sim \eta$ when ξ and η have the same distribution. For two sequences of positive random variables ξ_n and η_n, we write $\xi_n \asymp \eta_n$ if $\Pr(c\eta_n \leq \xi_n \leq C\eta_n) \to 1$ for some positive c and C.

$$\begin{aligned} T &= \frac{\beta^T \tilde{X}\tilde{X}^T\beta + 2\beta^T\tilde{X}\tilde{\epsilon} + \tilde{\epsilon}^T\tilde{\epsilon}}{\beta^T\tilde{X}(\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T\beta + 2\beta^T\tilde{X}(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon} + \tilde{\epsilon}^T(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon}} \\ &= \frac{A_1 + A_2 + A_3}{B_1 + B_2 + B_3}. \end{aligned} \tag{23}$$

4.1. Lemma

Lemma 1. *Suppose A is an $n \times n$ full rank symmetric matrix. And let*

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \tag{24}$$

where A_{11} is a real number, A_{12} is a $1 \times (n-1)$ matrix, A_{21} is a $(n-1) \times 1$ matrix and A_{22} is a $(n-1) \times (n-1)$ matrix. Denote $A_{11\cdot 2} = A_{11} - A_{12}A_{22}^{-1}A_{21}$. Then we have

$$(A^{-1})_{11} = A_{11\cdot 2}^{-1} \tag{25}$$

Lemma 2. *Suppose $B = \frac{1}{q}VV^T$ where V is an $p \times q$ random matrix composed of i.i.d. random variables with zero mean, unit variance and finite fourth moment. As $q \to \infty$ and $p/q \to c \in [0, +\infty)$, the largest and smallest nonzero eigenvalues of B converge almost surely to $(1+\sqrt{c})^2$ and $(1-\sqrt{c})^2$, respectively.*

Lemma 2 is known as the Bai-Yin's law [3].

Lemma 3. *Let $Z_1, \ldots, Z_{n+1}$ i.i.d. distributed as $N(0, I_p)$. $\Lambda = diag(\lambda_1, \ldots, \lambda_p)$, where $\lambda_1 \geq \cdots \lambda_r$ and $\lambda_{r+1} = \cdots = \lambda_p = \lambda$. $\limsup_{n\to\infty} \lambda_1/\lambda_r < \infty$, $\lambda_1/\sqrt{p} \to \infty$. Suppose $p = o(n^2)$. Denote $Z = (Z_1, \ldots, Z_n)$. Let $\hat{V}$ be the first r eigenvectors of $\Lambda^{1/2}ZZ^T\Lambda^{1/2}$, $V = (e_1, \ldots, e_r)$. Then*

$$Z_{n+1}^T\Lambda^{1/2}(VV^T - \hat{V}\hat{V}^T)\Lambda^{1/2}Z_{n+1} = o(\sqrt{p}) \tag{26}$$

Lemma 3 is from Wang Rui's paper.

Lemma 4. *Suppose $F_n(\cdot)$ and $F(\cdot)$ are distribution functions and $F_n \xrightarrow{L} F$, then*

$$\sup_x |F_n(x) - F(x)| \to 0. \tag{27}$$

See Exercise 3.2.9 of [4].

Lemma 5. *Suppose Z is an $p \times n$ ($p \geq n$) random matrix with all elements i.i.d. distributed as $N(0,1)$. Denote by $Z = U\Lambda V^T$ the singular value decomposition (SVD) of Z, where U is a $p \times n$ orthogonal matrix, Λ is an $n \times n$ diagonal matrix and V is an $n \times n$ orthogonal matrix. Then U, Λ and V are independent. (See, e.g., [5])*

Lemma 6. *Let A be an $n \times n$ symmetric positive semi-definite matrix with rank r. Denote by $A = P\Lambda P^T$ the spectral decomposition of A, where P is an $n \times r$ orthogonal matrix and $\Lambda = diag(\lambda_1, \ldots, \lambda_r)$ is an $r \times r$ diagonal matrix with $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_r > 0$. Then we have*

$$(A + I_n)^{-1} \geq I_n - PP^T \tag{28}$$

Proof. Let $\tilde{P}$ be an $n \times n$ orthogonal matrix such that P is the first r columns of $\tilde{P}$. And let $\tilde{\Lambda} = \mathrm{diag}(\lambda_1, \ldots, \lambda_r, 0, \ldots, 0)$ be an $n \times n$ matrix. Then $P\Lambda P^T = \tilde{P}\tilde{\Lambda}\tilde{P}^T$, and

$$\begin{aligned}
(A + I_n)^{-1} &= \tilde{P}(\tilde{\Lambda} + I_n)^{-1}\tilde{P}^T \\
&= \tilde{P}\mathrm{diag}((\lambda_1 + 1)^{-1}, \ldots, (\lambda_r + 1)^{-1}, 1, \ldots, 1)\tilde{P}^T \\
&\geq \tilde{P}\mathrm{diag}(0, \ldots, 0, 1, \ldots, 1)\tilde{P}^T \\
&= I_n - PP^T
\end{aligned} \tag{29}$$

□

4.2. circumstance 1

Assumption 1. $r = 0$.

Assumption 2. $n^2/p \to 0$.

4.2.1. First randomization of β

Independent of data, generate a random p dimensional orthonormal matrix O with Haar invariant distribution. And

$$T = \frac{(O\beta)^T O\tilde{X}(O\tilde{X})^T O\beta + 2(O\beta)^T \tilde{X}\tilde{\epsilon} + \tilde{\epsilon}^T\tilde{\epsilon}}{(O\beta)^T O\tilde{X}((O\tilde{X})^T O\tilde{X})^{-1}(O\tilde{X})^T\beta + 2(O\beta)^T O\tilde{X}((O\tilde{X})^T O\tilde{X})^{-1}\tilde{\epsilon} + \tilde{\epsilon}^T((O\tilde{X})^T O\tilde{X})^{-1}\tilde{\epsilon}} \tag{30}$$

Note that conditioning on O, $O\tilde{X}$ is a random matrix with each entry independently distributed as $N(0, \lambda)$. Hence O is independent of $O\tilde{X}$. Observe also that $O\beta/\|\beta\|$ is uniformly distributed on the unit ball. We can without loss of generality and assume that $\beta/\|\beta\|$ is uniformly distributed on the unit ball in (23).

4.2.2. Second randomization of β

Independent of data, generate $R > 0$ with R^2 distributed as χ^2_p. Then $\xi = R\beta/\|\beta\|$ distributed as $N_p(0, I_p)$. Note that conditioning on $\tilde{X}$, $\eta = (\tilde{X}^T\tilde{X})^{-1/2}\tilde{X}^T\xi$ is distributed as $N_{n-1}(0, I_{n-1})$. Hence η is independent of $\tilde{X}$.

Then

$$\begin{aligned} T &= \frac{(\|\beta\|/R)^2\xi^T\tilde{X}\tilde{X}^T\xi + 2(\|\beta\|/R)\xi^T\tilde{X}\tilde{\epsilon} + \tilde{\epsilon}^T\tilde{\epsilon}}{(\|\beta\|/R)^2\xi^T\tilde{X}(\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T\xi + 2(\|\beta\|/R)\xi^T\tilde{X}(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon} + \tilde{\epsilon}^T(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon}} \\ &= \frac{(\|\beta\|/R)^2\eta^T\tilde{X}^T\tilde{X}\eta + 2(\|\beta\|/R)\eta^T(\tilde{X}^T\tilde{X})^{1/2}\tilde{\epsilon} + \tilde{\epsilon}^T\tilde{\epsilon}}{(\|\beta\|/R)^2\eta^T\eta + 2(\|\beta\|/R)\eta^T(\tilde{X}^T\tilde{X})^{-1/2}\tilde{\epsilon} + \tilde{\epsilon}^T(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon}} \\ &= \frac{A_1 + A_2 + A_3}{B_1 + B_2 + B_3} \end{aligned} \tag{31}$$

4.2.3. Step 3: CLT

Similar to the derivation of the distribution of Hotelling's T^2 statistic.

Now we deal with

$$\frac{A_3}{B_3} = \frac{\tilde{\epsilon}^T\tilde{\epsilon}}{\tilde{\epsilon}^T(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon}} \tag{32}$$

Let O be an $(n-1)\times(n-1)$ orthogonal matrix satisfies

$$O\tilde{\epsilon} = \begin{pmatrix} \|\tilde{\epsilon}\| \\ 0 \\ \dots \\ 0 \end{pmatrix}.$$

Then

$$\frac{A_3}{B_3} = \frac{(O\tilde{\epsilon})^T O\tilde{\epsilon}}{(O\tilde{\epsilon})^T \left((\tilde{X}O^T)^T \tilde{X}O^T\right)^{-1} O\tilde{\epsilon}}. \tag{33}$$

It can be seen that $\tilde{X}O^T$ has the same distribution as $\tilde{X}$ and is independent of O. We have

$$\frac{A_3}{B_3} \sim \frac{1}{((\tilde{X}^T\tilde{X})^{-1})_{11}}. \tag{34}$$

Apply lemma 1, we have

$$\frac{A_3}{B_3} \sim (\tilde{X}^T\tilde{X})_{11\cdot 2}. \tag{35}$$

Since $\tilde{X}^T\tilde{X} \sim \mathrm{Wishart}_{n-1}(\lambda I_{n-1}, p)$, $(\tilde{X}^T\tilde{X})_{11\cdot 2} \sim \lambda\chi^2_{p-n+2}$. Hence $A_3/B_3 \asymp p$ and

$$\frac{A_3/B_3 - \lambda(p-n+2)}{\lambda\sqrt{2(p-n+2)}} \xrightarrow{\mathcal{L}} N(0,1), \tag{36}$$

by CLT.

Similar technique can deal with A_1/B_1:

$$\frac{A_1}{B_1} = \frac{\eta^T\tilde{X}^T\tilde{X}\eta}{\eta^T\eta} \sim (\tilde{X}^T\tilde{X})_{11} \sim \lambda\chi^2_p. \tag{37}$$

Hence $A_1/B_1 \asymp p$ and

$$\frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}} \xrightarrow{\mathcal{L}} N(0,1), \tag{38}$$

by CLT.

4.2.4. step 4

It's obvious that $A_3 \asymp n$ and $B_1 \asymp \frac{n}{p}\|\beta\|^2$. We already have $A_1/B_1 \asymp p$ and $A_3/B_3 \asymp p$. It follows that $A_1 \asymp n\|\beta\|^2$ and $B_3 \asymp n/p$. And

$$\begin{aligned}
A_2 &= O_P(\|\beta\|/\sqrt{p})\eta^T(\tilde{X}^T\tilde{X})^{1/2}\tilde{\epsilon} \\
&= O_P(\|\beta\|/\sqrt{p})\sqrt{\eta^T(\tilde{X}^T\tilde{X})\eta} \\
&= O_P(\|\beta\|/\sqrt{p})O_P(\sqrt{np}) \\
&= O_P(\sqrt{n}\|\beta\|),
\end{aligned} \tag{39}$$

$$\begin{aligned}
B_2 &= O_P(\|\beta\|/\sqrt{p})\eta^T(\tilde{X}^T\tilde{X})^{-1/2}\tilde{\epsilon} \\
&= O_P(\|\beta\|/\sqrt{p})\sqrt{\eta^T(\tilde{X}^T\tilde{X})^{-1}\eta} \\
&= O_P(\|\beta\|/\sqrt{p})O_P(\sqrt{n/p}) \\
&= O_P(\frac{\sqrt{n}}{p}\|\beta\|).
\end{aligned} \tag{40}$$

We can deduce that: If $\|\beta\|^2 \to 0$, then

$$T = \frac{\tilde{\epsilon}^T\tilde{\epsilon}}{\tilde{\epsilon}^T(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon}}(1 + o_P(1)), \tag{41}$$

and $T/(\lambda p) \xrightarrow{P} 1$. If $\|\beta\|^2 \to \infty$, then

$$T = \frac{\eta^T\tilde{X}^T\tilde{X}\eta}{\eta^T\eta}(1 + o_P(1)), \tag{42}$$

and $T/(\lambda p) \xrightarrow{P} 1$.

4.2.5. Step 5

If $\|\beta\|^2 \to 0$, we have

$$\begin{aligned}
&\Big|\frac{T-\lambda p}{\lambda\sqrt{2p}} - \frac{A_3/B_3-\lambda p}{\lambda\sqrt{2p}}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{A_1+A_2+A_3}{B_1+B_2+B_3} - \frac{A_3}{B_3}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{(A_1+A_2)B_3-(B_1+B_2)A_3}{(B_1+B_2+B_3)B_3}\Big| \\
&= \frac{O_P(1)}{\lambda\sqrt{2p}}\Big|\frac{(O_P(n\|\beta\|^2)+O_P(\sqrt{n}\|\beta\|))O_P(\frac{n}{p}) - (O_P(\frac{n}{p}\|\beta\|^2)+O_P(\frac{\sqrt{n}}{p}\|\beta\|))O_P(n)}{n^2/p^2}\Big| \\
&= O_P(\sqrt{p}\|\beta\|^2) + O_P(\frac{\sqrt{p}}{\sqrt{n}}\|\beta\|)
\end{aligned} \tag{43}$$

Hence if $\sqrt{p}\|\beta\|^2 \to 0$ and $\frac{p}{n}\|\beta\|^2 \to 0$, CLT holds.

On the other hand. If $\|\beta\|^2 \to \infty$, we have

$$\begin{aligned}
&\Big|\frac{T-\lambda p}{\lambda\sqrt{2p}} - \frac{A_1/B_1-\lambda p}{\lambda\sqrt{2p}}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{A_1+A_2+A_3}{B_1+B_2+B_3} - \frac{A_1}{B_1}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{(A_2+A_3)B_1-(B_2+B_3)A_1}{(B_1+B_2+B_3)B_1}\Big| \\
&= \frac{O_P(1)}{\lambda\sqrt{2p}}\Big|\frac{(O_P(\sqrt{n}\|\beta\|)+O_P(n))O_P(\frac{n}{p}\|\beta\|^2) - (O_P(\frac{\sqrt{n}}{p}\|\beta\|)+O_P(\frac{n}{p}))O_P(n\|\beta\|^2)}{\frac{n^2}{p^2}\|\beta\|^4}\Big| \\
&= O_P(\frac{\sqrt{p}}{\sqrt{n}}\|\beta\|^{-1}) + O_P(\sqrt{p}\|\beta\|^{-2})
\end{aligned} \tag{44}$$

Hence if $\frac{n}{p}\|\beta\|^2 \to \infty$ and $\frac{1}{\sqrt{p}}\|\beta\|^2 \to \infty$, CLT holds.

4.3. circumstance 2

Assumption 3. $P_1^T\beta = 0$.

$$
\begin{aligned}
T &= \frac{\beta^T\tilde{X}\tilde{X}^T\beta + 2\beta^T\tilde{X}\tilde{\epsilon} + \tilde{\epsilon}^T\tilde{\epsilon}}{\beta^T\tilde{X}\big(\tilde{X}^T\tilde{X}\big)^{-1}\tilde{X}^T\beta + 2\beta^T\tilde{X}\big(\tilde{X}^T\tilde{X}\big)^{-1}\tilde{\epsilon} + \tilde{\epsilon}^T\big(\tilde{X}^T\tilde{X}\big)^{-1}\tilde{\epsilon}} \\
&= \frac{\beta^T P_2 P_2^T\tilde{X}\tilde{X}^T P_2 P_2^T\beta + 2\beta^T P_2 P_2^T\tilde{X}\tilde{\epsilon} + \tilde{\epsilon}^T\tilde{\epsilon}}{\beta^T P_2 P_2^T\tilde{X}\big(\tilde{X}^T\tilde{X}\big)^{-1}\tilde{X}^T P_2 P_2^T\beta + 2\beta^T P_2 P_2^T\tilde{X}\big(\tilde{X}^T\tilde{X}\big)^{-1}\tilde{\epsilon} + \tilde{\epsilon}^T\big(\tilde{X}^T\tilde{X}\big)^{-1}\tilde{\epsilon}} \\
&= \frac{A_1 + A_2 + A_3}{B_1 + B_2 + B_3}
\end{aligned} \tag{45}
$$

4.3.1. Step 1

Like before, we have $A_3/B_3 \sim (\tilde{X}^T\tilde{X})_{11\cdot 2}$. Denote by $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_p)$. Let $Z = (Z_1, \ldots, Z_p)$ be a $n-1 \times p$ matrix with all elements independently distributed as $N(0,1)$. Let $Z_{(1)}$ and $Z_{(2)}$ be the first 1 row and last $n-2$ rows of Z, that is

$$
Z = \begin{pmatrix} Z_{(1)} \\ Z_{(2)} \end{pmatrix}.
$$

Then

$$
\begin{aligned}
\tilde{X}^T\tilde{X} &\sim Z\Lambda Z^T \\
&= \begin{pmatrix} Z_{(1)}\Lambda Z_{(1)}^T & Z_{(1)}\Lambda Z_{(2)}^T \\ Z_{(2)}\Lambda Z_{(1)}^T & Z_{(2)}\Lambda Z_{(2)}^T \end{pmatrix}.
\end{aligned} \tag{46}
$$

Hence

$$
\begin{aligned}
T &\sim Z_{(1)}\Lambda Z_{(1)}^T - Z_{(1)}\Lambda Z_{(2)}^T\big(Z_{(2)}\Lambda Z_{(2)}^T\big)^{-1} Z_{(2)}\Lambda Z_{(1)}^T \\
&= Z_{(1)}\Lambda^{1/2}\big(I_p - \Lambda^{1/2} Z_{(2)}^T\big(Z_{(2)}\Lambda Z_{(2)}^T\big)^{-1} Z_{(2)}\Lambda^{1/2}\big)\Lambda^{1/2} Z_{(1)}^T \\
&\leq Z_{(1)}\Lambda^{1/2}\big(I_p - \hat{V}\hat{V}^T\big)\Lambda^{1/2} Z_{(1)}^T.
\end{aligned} \tag{47}
$$

We require $p = o(n^2)$. The principal space is $V = (e_1, \ldots, e_r)$. Then

$$
Z_{(1)}\Lambda^{1/2}\big(VV^T - \hat{V}\hat{V}^T\big)\Lambda^{1/2} Z_{(1)}^T = o(\sqrt{p}) \tag{48}
$$

Note that

$$
Z_{(1)}\Lambda^{1/2}\big(I - VV^T\big)\Lambda^{1/2} Z_{(1)}^T \sim \lambda\chi^2_{p-r} \tag{49}
$$

Hence $T \leq \lambda\chi^2_{p-r} + o(\sqrt{p})$.

On the other hand, the eigenvalues of $\Lambda^{1/2}\big(I_p - \Lambda^{1/2}Z_{(2)}^T(Z_{(2)}\Lambda Z_{(2)}^T)^{-1}Z_{(2)}\Lambda^{1/2}\big)\Lambda^{1/2}$ is no less than $I_p - \Lambda^{1/2}Z_{(2)}^T(Z_{(2)}\Lambda Z_{(2)}^T)^{-1}Z_{(2)}\Lambda^{1/2}$. Hence $T \geq \lambda\chi^2_{p-n+2}$.

Hence $A_3/B_3 \asymp p$ if $p/n \to \infty$.

4.3.2. Step 2

Note that $P_2^T\tilde{X}$ is an $(p-r)\times(n-1)$ matrix with all elements independently distributed as $N(0,\lambda)$.

$A_1 \asymp n\|P_2^T\beta\|^2$, $A_2 = O_P(\sqrt{n}\|P_2^T\beta\|)$, $A_3 \asymp n$.

$B_3 \asymp n/p$.

As for B_1,

$$\begin{aligned} B_1 &\leq \beta^T P_2 P_2^T \tilde{X}(\tilde{X}^T P_2 P_2^T \tilde{X})^{-1}\tilde{X}^T P_2 P_2^T \beta \\ &\asymp \frac{n-1}{p-r}\|P_2^T\beta\|^2 \end{aligned} \tag{50}$$

To get the lower bound, let $P_2^T\tilde{X} = U_2 D_2 V_2^T$ be the SVD of $P_2^T\tilde{X}$, where U_2 is a $(p-r)\times(n-1)$ orthonormal matrix, D_2 is a $(n-1)\times(n-1)$ diagonal matrix and V_2 is a $(n-1)\times(n-1)$ orthonormal matrix. Then

$$\begin{aligned} B_1 &= \beta^T P_2 P_2^T \tilde{X}(\tilde{X}^T P_1 P_1^T \tilde{X} + \tilde{X}^T P_2 P_2^T \tilde{X})^{-1}\tilde{X}^T P_2 P_2^T \beta \\ &= \beta^T P_2 U_2 D_2 V_2^T (\tilde{X}^T P_1 P_1^T \tilde{X} + V_2 D_2^2 V_2^T)^{-1} V_2 D_2 U_2^T P_2^T \beta \\ &= \beta^T P_2 U_2 (D_2^{-1} V_2^T \tilde{X}^T P_1 P_1^T \tilde{X} V_2 D_2^{-1} + I_{n-1})^{-1} U_2^T P_2^T \beta \end{aligned} \tag{51}$$

Note that U_2 is independent of $(V_2, D_2, P_1^T\tilde{X})$, and

$$(D_2^{-1}V_2^T\tilde{X}^T P_1 P_1^T \tilde{X} V_2 D_2^{-1} + I_{n-1})^{-1} \geq I_{n-1} - U^* U^{*T} \tag{52}$$

where U^* is the first r eigenvectors of $D_2^{-1}V_2^T\tilde{X}^T P_1 P_1^T \tilde{X} V_2 D_2^{-1}$ and is independent of U_2. Note also that U_2 is of Haar distribution. Hence

$$\begin{aligned} B_1 &\geq \beta^T P_2 U_2 (I_{n-1} - U^* U^{*T}) U_2^T P_2^T \beta \\ &\asymp \frac{n-1-r}{p-r}\|P_2^T\beta\|^2 \end{aligned} \tag{53}$$

$$\begin{aligned} \text{Upper-Lower} &\leq \beta^T P_2 U_2 U^* U^{*T} U_2^T P_2^T \beta \\ &\asymp \frac{r}{p-r}\|P_2^T\beta\|^2 \end{aligned} \tag{54}$$

Hence

$$\begin{aligned} B_1 &= \beta^T P_2 P_2^T \tilde{X}(\tilde{X}^T P_2 P_2^T \tilde{X})^{-1} \tilde{X}^T P_2 P_2^T \beta + O_p(\frac{r}{p-r}\|P_2^T\beta\|^2) \\ &= \beta^T P_2 P_2^T \tilde{X}(\tilde{X}^T P_2 P_2^T \tilde{X})^{-1} \tilde{X}^T P_2 P_2^T \beta(1+O_P(1/n)) \end{aligned} \tag{55}$$

$$\begin{aligned} B_2 &= O_P(1)\sqrt{\beta^T P_2 P_2^T \tilde{X}(\tilde{X}^T \tilde{X})^{-2} \tilde{X}^T P_2 P_2^T \beta} \\ &\le \lambda_{\min}(\tilde{X}^T\tilde{X})^{-1/2} O_P(1)\sqrt{\beta^T P_2 P_2^T \tilde{X}(\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T P_2 P_2^T \beta} \end{aligned} \tag{56}$$

$$\lambda_{\min}(\tilde{X}^T\tilde{X}) \ge \lambda_{\min}(\tilde{X}^T P_2 P_2^T \tilde{X}) \asymp p - r \tag{57}$$

Hence $B_2 = O_P(\frac{\sqrt{n}}{p}\|P_2^T\beta\|)$.

Hence the similar law of large number and CLT holds.

4.3.3. Step 3

$$\frac{A_1}{B_1} \sim \frac{\chi_p^2}{1+O_P(1/n)} = \lambda\chi_p^2(1+O_P(1/n)) \tag{58}$$

Hence if $\|P_2^T\beta\| \to \infty$ or $\|P_2^T\beta\| \to 0$,

$$\frac{T}{\lambda p} \xrightarrow{P} 1. \tag{59}$$

We have

$$\frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}} \sim \frac{\chi_p^2(1+O_P(1/n)) - p}{\sqrt{2p}} \xrightarrow{\mathcal{L}} N(0,1), \tag{60}$$

if $p = o(n^2)$.

Because $A_3/B_3 \le \lambda\chi_{p-r}^2 + o(\sqrt{p}) \le \lambda\chi_p^2 + o(\sqrt{p})$ (if $p = o(n^2)$). We have

$$\frac{A_3/B_3 - \lambda p}{\lambda\sqrt{2p}} \le \frac{\chi_p^2 + o(\sqrt{p}) - p}{\sqrt{2p}} \xrightarrow{\mathcal{L}} N(0,1). \tag{61}$$

If $\|P_2^T\beta\|^2 \to 0$, we have

$$
\begin{aligned}
&\Big|\frac{T-\lambda p}{\lambda\sqrt{2p}} - \frac{A_3/B_3-\lambda p}{\lambda\sqrt{2p}}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{A_1+A_2+A_3}{B_1+B_2+B_3} - \frac{A_3}{B_3}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{(A_1+A_2)B_3-(B_1+B_2)A_3}{(B_1+B_2+B_3)B_3}\Big| \\
&= \frac{O_P(1)}{\lambda\sqrt{2p}}\Big|\frac{(O_P(n\|P_2^T\beta\|^2)+O_P(\sqrt{n}\|P_2^T\beta\|))O_P(\frac{n}{p})-(O_P(\frac{n}{p}\|P_2^T\beta\|^2)+O_P(\frac{\sqrt{n}}{p}\|P_2^T\beta\|))O_P(n)}{n^2/p^2}\Big| \\
&= O_P(\sqrt{p}\|P_2^T\beta\|^2)+O_P(\frac{\sqrt{p}}{\sqrt{n}}\|P_2^T\beta\|)
\end{aligned}
\tag{62}
$$

Hence if $\sqrt{p}\|P_2^T\beta\|^2 \to 0$ and $\frac{p}{n}\|P_2^T\beta\|^2 \to 0$, CLT holds.

On the other hand. If $\|P_2^T\beta\|^2 \to \infty$, we have

$$
\begin{aligned}
&\Big|\frac{T-\lambda p}{\lambda\sqrt{2p}} - \frac{A_1/B_1-\lambda p}{\lambda\sqrt{2p}}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{A_1+A_2+A_3}{B_1+B_2+B_3} - \frac{A_1}{B_1}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{(A_2+A_3)B_1-(B_2+B_3)A_1}{(B_1+B_2+B_3)B_1}\Big| \\
&= \frac{O_P(1)}{\lambda\sqrt{2p}}\Big|\frac{(O_P(\sqrt{n}\|P_2^T\beta\|)+O_P(n))O_P(\frac{n}{p}\|P_2^T\beta\|^2)-(O_P(\frac{\sqrt{n}}{p}\|P_2^T\beta\|)+O_P(\frac{n}{p}))O_P(n\|P_2^T\beta\|^2)}{\frac{n^2}{p^2}\|P_2^T\beta\|^4}\Big| \\
&= O_P(\frac{\sqrt{p}}{\sqrt{n}}\|P_2^T\beta\|^{-1})+O_P(\sqrt{p}\|P_2^T\beta\|^{-2})
\end{aligned}
\tag{63}
$$

Hence if $\frac{n}{p}\|P_2^T\beta\|^2 \to \infty$ and $\frac{1}{\sqrt{p}}\|P_2^T\beta\|^2 \to \infty$, CLT holds.

4.4. Consistency of Test

β from normal distribution. Then consistency can be proved. Assume that $\beta \sim N(0, \sigma_\beta^2 I_p)$. Then $\gamma = (\tilde{X}^T\tilde{X})^{-1/2}\tilde{X}^T\beta \sim N(0, \sigma_\beta^2 I_{n-1})$.

$$
\begin{aligned}
T &= \frac{\beta^T\tilde{X}\tilde{X}^T\beta + 2\beta^T\tilde{X}\tilde{\epsilon} + \tilde{\epsilon}^T\tilde{\epsilon}}{\beta^T\tilde{X}(\tilde{X}^T\tilde{X})^{-1}\tilde{X}^T\beta + 2\beta^T\tilde{X}(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon} + \tilde{\epsilon}^T(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon}} \\
&= \frac{\gamma^T\tilde{X}^T\tilde{X}\gamma + 2\gamma^T(\tilde{X}^T\tilde{X})^{1/2}\tilde{\epsilon} + \tilde{\epsilon}^T\tilde{\epsilon}}{\gamma^T\gamma + 2\gamma^T(\tilde{X}^T\tilde{X})^{-1/2}\tilde{\epsilon} + \tilde{\epsilon}(\tilde{X}^T\tilde{X})^{-1}\tilde{\epsilon}} \\
&= \frac{A_1+A_2+A_3}{B_1+B_2+B_3}
\end{aligned}
\tag{64}
$$

$A_1 \sim \|\gamma\|^2 \sum_{i=1}^p \lambda_i \chi_1^2 \asymp \|\gamma\|^2 (p+\lambda_1) \asymp \sigma_\beta^2 n(p+\lambda_1)$. $A_2 = O_P(\sqrt{A_1})$. $A_3 \asymp n$.

$B_1 \asymp \sigma_\beta^2 n$. $B_3 \leq \tilde{\epsilon}(\tilde{X}^T P_2 P_2^T \tilde{X})^{-1} \tilde{\epsilon} \asymp n/p$. $B_2 = O_P(\sqrt{B_3}\sigma_\beta)$.

$A_1/B_1 \sim \sum_{i=1}^p \lambda_i \chi_1^2$. Hence

$$\mathbb{P}\Big(\frac{A_1/B_1 - (p-r)\lambda}{\lambda\sqrt{2(p-r)}} \geq \Phi^{-1}(1-\alpha)\Big) \sim \mathbb{P}\Big(N(0,1) \geq \Phi^{-1}(1-\alpha) - \frac{\sum_{i=1}^r \lambda_i \chi_i^2}{\lambda\sqrt{2(p-r)}}\Big)$$
$$= \mathrm{E}[\Phi\Big(-\Phi^{-1}(1-\alpha) + \frac{\sum_{i=1}^r \lambda_i \chi_i^2}{\lambda\sqrt{2(p-r)}}\Big)] \tag{65}$$

And note that if $p\sigma_\beta^2 \to \infty$,

$$\begin{aligned}
&\Big|\frac{T-\lambda p}{\lambda\sqrt{2p}} - \frac{A_1/B_1 - \lambda p}{\lambda\sqrt{2p}}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{A_1+A_2+A_3}{B_1+B_2+B_3} - \frac{A_1}{B_1}\Big| \\
&= \frac{1}{\lambda\sqrt{2p}}\Big|\frac{(A_2+A_3)B_1 - (B_2+B_3)A_1}{(B_1+B_2+B_3)B_1}\Big| \\
&= \frac{O_P(1)}{\lambda\sqrt{2p}}\Big|\frac{(O_P(\sigma_\beta\sqrt{n(p+\lambda_1)}) + O_P(n))O_P(\sigma_\beta^2 n) - (O_P(\sigma_\beta\frac{\sqrt{n}}{\sqrt{p}}) + O_P(\frac{n}{p}))O_P(\sigma_\beta^2 n(p+\lambda_1))}{\sigma_\beta^4 n^2}\Big| \\
&= O_P(\frac{p+\lambda_1}{\sigma_\beta\sqrt{np}}) + O_P(\frac{p+\lambda_1}{\sigma_\beta^2 p^{3/2}})
\end{aligned} \tag{66}$$

Hence if

$$\frac{np^2 + p^{5/2} + \lambda_1 p^{3/2}}{(p+\lambda_1)^2}\sigma_\beta^2 \to \infty \tag{67}$$

Then Power function holds.

5. Simulation Results

References

[1] T. T. Cai, Z. Ma, Y. Wu, Sparse pca: Optimal rates and adaptive estimation, Annals of Statistics 41 (6) (2012) 3074–3110.

[2] J. Zhao, X. Xu, A generalized likelihood ratio test for normal mean when p is greater than n, Computational Statistics & Data Analysis.

[3] Z. D. Bai, Y. Q. Yin, Limit of the smallest eigenvalue of a large dimensional sample covariance matrix, Annals of Probability 21 (3) (1993) 1275–1294.

[4] R. Durrett, Probability : theory and examples, Journal of the American Statistical Association 87 (418) (2010) 586.

[5] M. L. Eaton, Multivariate statistics: A vector space approach 80 (392) (1983) 72.